

Functional integration with “automorphic” boundary conditions and correlators of z -components of spins in the XY and XX Heisenberg chains

C. MALYSHEV

*V. A. Steklov Institute of Mathematics,
St.-Petersburg Department,
Fontanka 27, St.-Petersburg, 191023, RUSSIA
E-mail: malyshev@pdmi.ras.ru*

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Abstract

Representations for the generating functionals of static correlators of z -components of spins in the XY and XX Heisenberg spin chains are obtained in the form of sums of the fermionic functional integrals. The peculiarity of the functional integrals in question is because of the fact that the integration variables depend on the imaginary time “automorphically”. In other words, the integration variables are multiplied with a certain complex number when the imaginary time is shifted by a period. Therefore, the corresponding boundary conditions at the ends of the imaginary time segment are not of the form corresponding to fermionic, or bosonic, variables taken in the Matsubara representation at nonzero temperature. In fact, one part of sites of the models corresponds to the integration variables which are subjected to the unusual boundary conditions, while the variables on the other sites depend on the imaginary time conventionally, i.e., as fermions (or bosons). Thus a situation, when an “automorphic” boundary condition is the same for all sites of a chain spin model, is generalized. The results of the functional integration are obtained in the form of determinants of the matrix operators which are regularized by means of the generalized zeta-function approach. The partition functions of the models and certain correlation functions at nonzero temperature are obtained explicitly thus demonstrating correctness of the functional integral representations proposed.

1 Introduction

The correlation functions of quantum models that are solvable via the Bethe ansatz method [1] can be represented, in the thermodynamic limit, as the Fredholm determinants of certain linear integral operators. One of such *determinant* representations has been obtained in [2] for an equal-time correlator of one-dimensional model of “impenetrable” bosons, which are described by the quantum non-linear Schrödinger equation with infinite coupling. This result has been generalized to the case of correlators with different time arguments [3], and also to the case of the XX spin $1/2$ Heisenberg chain [4]. The determinant representations of the correlation functions allow to deduce the non-linear integrable partial differential equations for the correlators [1], [5]. Various determinant representations have been deduced in [6], [7], [8], [9], [10], [11] (see also Refs. in [1]), for instance, for the temperature correlators of quantum non-linear Schrödinger equation and for XXX and XXZ spin $1/2$ Heisenberg chains. It should be noticed that XX and XY Heisenberg models still continue to attract attention [12], [13], [14], and the multiple integral representations as well as the determinant representations for the correlators in these models are also actively studied [15], [16]. Multiple integration over a set of the Grassmann coherent states is used in [11], [16].

In its turn, *functional integration* (or *path integration*) technique can be used to calculate the correlation functions in various quantum models [17], [18], [19], [20], [21], [22]. The present paper is based on [23], where an approach has been proposed to represent the generating functional of correlators of z -components of spins, as well as the partition function, in the Heisenberg XX -model by means of functional integrals defined on the variables subjected to, so-called, “automorphic” boundary conditions.

Approach [23] is based on a technical consideration carried out in Ref.[24] (see also [25]) which is concerned with the index theory and supersymmetric quantum mechanical systems. Path integration is used in [24] to evaluate traces of those supersymmetric quantum mechanical operators which appear in dealing with various differential geometric indices. In this respect, the Ref.[24] follows [18], [26], for the usage of holomorphic representation of functional integrals to propose an example of path integral defined on the trajectories subjected to non-conventional boundary conditions at the ends of the segment of imaginary time.

It has been shown in [23] that the generating functional of static correlators of z -components of local spins in the XX Heisenberg magnet can also be represented by means of the (Gaussian) functional integrals which are defined on the trajectories depending on the imaginary time non-conventionally in the sense of [24]. In other words, the variables of the functional integration are multiplied with a certain complex number when the imaginary time is shifted by a period, i.e., the variables behave “automorphically” under such shifts. More precisely, the path integrals considered in [23] are defined for the set of variables a part of which is subjected to the “automorphic” boundary conditions, whereas the other part satisfy the standard requirements of the fermion/boson-type.

The point is that a trace of an operator exponential is evaluated in [23], and the quadratic operator in the exponent is defined only on the first m sites of the model in question ($m \leq M$, M is the total number of sites). Remind that the XX model considered in [23] can equivalently be handled in the representation of free fermions. Eventually, after a passage from a multiple integral over the Grassmann coherent states to the continual (i.e., functional) one, it turns out to be possible to define the integration domain so that

the integration variables are “automorphic” in the imaginary time on the first m sites, while they are (anti-)periodic on the other sites.

The interest to the functional integrals defined on the trajectories with “automorphic” dependence on the imaginary time can also be traced back to [27], [28]. An essential distinction between the formulations discussed in [23] and in [24], [27] consists in the fact that the “automorphic” boundary condition for the segment of the imaginary time turns out to be “inhomogeneous” spatially since it is valid only for a part of sites of the chain model in question. The dependence of the integration variables on the imaginary time in [24], [27] is the same for all sites.

The given paper continues [23], and it is concerned with carrying of the approach proposed to the XY Heisenberg magnet which is equivalent to quasi-free fermions (i.e., its Hamiltonian in the fermionic representation is diagonalized by the Bogoliubov transformation). It should be noticed that our path integral representations do not imply a straightforward implementation of the proposal [24]: a special restoration of invariance of the Lagrangian of the model in question under shifts of the imaginary time by a period is required. The method of zeta-regularization is used in what follows to handle the determinants obtained. The generating functional, as well as the partition function of the model, are calculated. Certain correlation functions at nonzero temperature are obtained explicitly. Thus it is demonstrated that the path integration approach proposed admits a considerable simplification and enough transparency for the problem in question.

From a physical viewpoint, basic ideas of *zeta-regularization* (ζ -regularization) have been formulated in [29], [30], [31], [32]. In mathematical literature, usage of ζ -regularization is usually traced to [33]. Zeta-regularization turned out to be rather useful in physics to calculate, say, the instanton determinants [34], [35], the Casimir energy on manifolds [36], [37], as well as the axial and conformal anomalies [38]. One should be referred to [31], [32], [33], [39] for exposition of ζ -regularization.

The paper is organized as follows. Section 2 contains outline of the problem and basic notations. The representation for the generating functionals of correlators of σ_n^z -operators (and also for the partition functions) in the form given by a combination of the fermionic functional integrals with “automorphic” boundary conditions is obtained in Section 3 (σ_n^z implies the Pauli matrix σ^z at n th site). Section 4 contains calculation of the functional integrals, i.e., obtaining of the answers in the determinant form. The most important formulas of ζ -regularization are given in Section 5. Moreover, the partition function of the XY (and, so, of the XX) model is calculated in Section 5 with the use of the generalized ζ -function in the series form. The generalized ζ -function in the form of a Mellin transform is defined in Section 6, and it is used to obtain the regularized answers in the form of determinants of finite-dimensional matrices which constitute, in their turn, the total generating functional. Differentiation of the integrals obtained with respect to a parameter is also considered in Section 6, and some concrete correlators are calculated. Reductions of the answers for the XY model to those of the XX model are verified. Discussion in Section 7 concludes the paper.

2 Outline of the model and notations

Let us consider the XY Heisenberg magnet of spin $1/2$ [40], [41] on a periodic chain with the total number of sites M (with even M). Let $Q(m)$ to denote an operator of number of

quasi-particles on the first m sites of the chain ($m \leq M$). We shall calculate an average of the operator exponential $\exp(\alpha Q(m))$ over the ground state of the model (our notations, though conventional, correspond to [4], [10], [11]),

$$G(\alpha, m) \equiv \langle \Phi_0 | e^{\alpha Q(m)} | \Phi_0 \rangle = \frac{\text{Tr}(e^{\alpha Q(m)} e^{-\beta H_{XY}})}{\text{Tr}(e^{-\beta H_{XY}})}, \quad \alpha \in \mathcal{C}, \quad (2.1)$$

where H_{XY} is the Hamiltonian of the XY model, β is inverse temperature ($\beta = 1/T$), and Tr means trace of operator. The vacuum average (2.1) plays the role of a generating functional of static correlators of third components of spins of the magnetic chains [4], [7], [10], [11], [15].

The Hamiltonian of the XY model has the form:

$$H = H_0 + \gamma H_1 - h S^z, \quad (2.2)$$

where

$$H_0 = -\frac{1}{2} \sum_{n=1}^M (\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+), \quad (2.3)$$

$$H_1 = -\frac{1}{2} \sum_{n=1}^M (\sigma_n^+ \sigma_{n+1}^+ + \sigma_n^- \sigma_{n+1}^-), \quad S^z = \frac{1}{2} \sum_{n=1}^M \sigma_n^z, \quad (2.4)$$

where S^z is the total spin, h is an external magnetic field ($h \geq 0$, [1], [4], [15]). The algebra of the Pauli spin operators on the sites, σ_n^α , $n \in \{1, \dots, M\}$, is defined by the commutation relations:

$$[\sigma_k^\alpha, \sigma_n^\beta] = 2i \delta_{kn} \epsilon^{\alpha\beta\gamma} \sigma_n^\gamma, \quad \sigma_n^\pm = (1/2)(\sigma_n^x \pm i\sigma_n^y),$$

where $\epsilon^{\alpha\beta\gamma}$ is the totally antisymmetric symbol, and the indices α, β, γ acquire the “values” x, y, z . Besides, the periodic boundary conditions are imposed: $\sigma_{n+M}^\alpha = \sigma_n^\alpha$, $\forall n$. Real parameter γ characterizes anisotropy: we obtain the XX Heisenberg magnet at $\gamma = 0$.

Let us use the Jordan–Wigner transformation from the variables σ_k^α to the canonical fermionic variables c_k, c_k^\dagger :

$$c_k = \exp\left(i\pi \sum_{n=1}^{k-1} \sigma_n^- \sigma_n^+\right) \sigma_k^+, \quad c_k^\dagger = \sigma_k^- \exp\left(-i\pi \sum_{n=1}^{k-1} \sigma_n^- \sigma_n^+\right). \quad (2.5)$$

The variables c_k, c_k^\dagger are subjected to the anti-commutation relations:

$$\{c_k, c_n\} = \{c_k^\dagger, c_n^\dagger\} = 0, \quad \{c_k, c_n^\dagger\} = \delta_{kn},$$

where the brackets $\{, \}$ imply anti-commutation. As a result of the transformation (2.5), the Hamiltonian (2.2)–(2.4) acquires the following form in the fermionic representation [42]:

$$H = H^+ P^+ + H^- P^-, \quad (2.6)$$

$$\begin{aligned} H^\pm = & -\frac{1}{2} \sum_{k=1}^M \left[c_k^\dagger c_{k+1} + c_{k+1}^\dagger c_k + \gamma (c_{k+1} c_k + c_k^\dagger c_{k+1}^\dagger) \right] \\ & + h \sum_{k=1}^M c_k^\dagger c_k - hM/2. \end{aligned} \quad (2.7)$$

The Hamiltonians H^\pm (2.7) look similar each to other except for the choice of the spatial boundary condition for each of them: the superscripts \pm are chosen in correspondence with the boundary conditions for c_k, c_k^\dagger in the form:

$$c_{M+1} = \mp c_1, \quad c_{M+1}^\dagger = \mp c_1^\dagger. \quad (2.8)$$

We have got in new variables: $Q(m) = \sum_{k=1}^m c_k^\dagger c_k$ is the number operator of quasi-particles on first m sites, the total number of quasi-particles is $\mathcal{N} \equiv Q(M)$, and the projectors P^\pm in (2.6) are defined conventionally: $P^\pm = (1/2)(1 \pm (-1)^\mathcal{N})$ [42]. Operator \mathcal{N} commutes only with H_0 (2.3) and S^z (2.4) but not with H_1 (2.4). The parity operator $(-1)^\mathcal{N}$ anti-commutes with c_k^\dagger and c_k , and it commutes with H .

As a result, we obtain the following representation for $G(\alpha, m)$ (2.1) [11]:

$$\begin{aligned} G(\alpha, m) &= (2Z)^{-1} (G_F^+ Z_F^+ + G_F^- Z_F^- + G_B^+ Z_B^+ - G_B^- Z_B^-), \\ G_F^\pm Z_F^\pm &\equiv \text{Tr} \left(e^{\alpha Q(m)} e^{-\beta H^\pm} \right), \\ G_B^\pm Z_B^\pm &\equiv \text{Tr} \left(e^{\alpha Q(m)} (-1)^\mathcal{N} e^{-\beta H^\pm} \right) \end{aligned} \quad (2.9)$$

(in what follows we omit the subscript XY in the Hamiltonians). For the partition function Z we have got:

$$\begin{aligned} Z &= (1/2)(Z_F^+ + Z_F^- + Z_B^+ - Z_B^-), \\ Z_F^\pm &= \text{Tr} (e^{-\beta H^\pm}), \quad Z_B^\pm = \text{Tr} \left((-1)^\mathcal{N} e^{-\beta H^\pm} \right). \end{aligned} \quad (2.10)$$

The following observation is discussed in Ref.[24], which is concerned with the index theory and supersymmetric quantum mechanics. Let a, a^\dagger be some fermionic canonical operators. Let us consider $\mathcal{U}(1)$ -operator $Q_\vartheta \equiv \exp(i\vartheta a^\dagger a)$, which acts on a, a^\dagger as follows:

$$Q_\vartheta a Q_\vartheta^\dagger = e^{-i\vartheta} a, \quad Q_\vartheta a^\dagger Q_\vartheta^\dagger = e^{i\vartheta} a^\dagger.$$

When calculating the trace $\text{Tr} (Q_\vartheta \exp(-\beta H))$ in the path integral representation (H is a Hamiltonian), it turns out to be rather natural to come to a path integral over the variable subjected to the “automorphic” boundary condition:

$$\xi(\tau) = -e^{i\vartheta} \xi(\tau + \beta), \quad (2.11)$$

where τ is imaginary time, $\tau \in [0, \beta]$. Indeed, Eq. (2.11) reminds the definition of an automorphic function (automorphic form, [43], [44]):

$$g^* f \equiv f(gu) = r(g) f(u),$$

where $f(u)$ is an appropriate function (form), g is an element of a group of transformations acting on the argument u (thus generating an action of g^* on f), and $r(g)$ denotes a representation of g^* . Thus, Eq. (2.11) implies that the integration variable is transformed accordingly to a nontrivial representation of $\mathcal{U}(1)$ when τ is shifted by the period β . Other physical (quantum-statistical, in fact) examples of “automorphic” boundary conditions at the ends of the segment $[0, \beta] \ni \tau$ can be found in [27], where spin $1/2$ and spin 1 chain models are studied by the method of functional integration.

It is not difficult to note that operator $\exp(\alpha Q(m))$ behaves analogously:

$$e^{\alpha Q(m)} c_n e^{-\alpha Q(m)} = \begin{cases} e^{-\alpha} c_n, & 1 \leq n \leq m, \\ c_n, & m < n \leq M, \end{cases} \quad (2.12)$$

and it is suggestive to use the idea of [24] when calculating $G_F^\pm Z_F^\pm$, $G_B^\pm Z_B^\pm$ (2.9). The “automorphic” condition arises for all sites in the models considered in [24]. The peculiarity due to (2.12) is concerned with $m \leq M$, and the “automorphic” condition is expected to appear only for a part of sites.

To conclude the section, let us define the coherent states using the fermionic operators c_n , c_n^\dagger which possess the Fock vacuum $|0\rangle$:

$$c_n |0\rangle = \langle 0| c_n^\dagger = 0, \quad \forall n \in \{1, \dots, M\}, \quad \langle 0|0\rangle = 1.$$

Namely, we define the states

$$\begin{aligned} |x(a)\rangle &= \exp \left\{ \sum_{k=1}^M c_k^\dagger x_k(a) \right\} |0\rangle \equiv \exp(c^\dagger x(a)) |0\rangle, \\ \langle x^*(a)| &= \langle 0| \exp \left\{ \sum_{k=1}^M x_k^*(a) c_k \right\} \equiv \langle 0| \exp(x^*(a) c), \end{aligned} \quad (2.13)$$

where a is discrete index running from 1 to N , and the shorthand notations are used: $\sum_{k=1}^M c_k^\dagger x_k \equiv c^\dagger x$, $\prod_{k=1}^M dx_k \equiv dx$, etc. In fact, N independent coherent states are defined which are labeled by independent complex-valued Grassmann parameters $x_k^*(a)$, $x_k(a)$. The following relations hold for the states (2.13):

$$\begin{aligned} c_k |x(a)\rangle &= x_k(a) |x(a)\rangle, \quad \langle x^*(a)| c_k^\dagger = \langle x^*(a)| x_k^*(a), \\ \langle x^*(a)| x(a)\rangle &= \exp(x^*(a) x(a)). \end{aligned}$$

3 The functional integral

Let us turn to the problem of rewriting $G_F^\pm Z_F^\pm$, $G_B^\pm Z_B^\pm$ (2.9) and Z_F^\pm , Z_B^\pm (2.10) in the form of functional integrals. For definiteness, let us consider $G_F^\pm Z_F^\pm$:

$$G_F^\pm Z_F^\pm = \int dz dz^* e^{z^* z} \langle z^* | e^{\alpha Q(m)} e^{-\beta H^\pm} | z \rangle, \quad (3.1)$$

where it is understood that the trace of operator is calculated as the integral over the anti-commuting variables [26], [45], and the coherent states $\langle z^*|$, $|z\rangle$ are defined analogously to (2.13):

$$\langle z^*| = \langle 0| \exp(z^* c), \quad |z\rangle = \exp(c^\dagger z) |0\rangle.$$

In order to go over to the path integral, let us divide the segment $[0, \beta]$ into N parts of the length β/N , and let us represent $\exp(-\beta H^\pm)$ as a product of N identical exponentials. Inserting N decompositions of unity between the exponentials, let us transform (3.1) into

$$\begin{aligned} G_F^\pm Z_F^\pm &= \int dz dz^* \prod_{a=1}^N dx^*(a) dx(a) \exp \left(z^* z - \sum_{a=1}^N x^*(a) x(a) \right) \\ &\times \langle z^* | e^{\alpha Q(m)} | x(1) \rangle \langle x^*(1) | e^{-\frac{\beta}{N} H^\pm} | x(2) \rangle \dots \langle x^*(N) | e^{-\frac{\beta}{N} H^\pm} | z \rangle, \end{aligned} \quad (3.2)$$

where $|x(a)\rangle$ and $\langle x^*(a)|$ are defined in (2.13).

Using the properties of the coherent states we evaluate the following averages:

$$\langle z^* | e^{\alpha Q(m)} | x(1) \rangle = \exp \left(e^\alpha \sum_{k=1}^m z_k^* x_k(1) + \sum_{k=m+1}^M z_k^* x_k(1) \right), \quad (3.3)$$

$$\begin{aligned} & \langle x^*(a) | e^{-\frac{\beta}{N} H^\pm} | x(a+1) \rangle \underset{N \gg 1}{\simeq} \\ & \simeq \exp \left(x^*(a) x(a+1) - \frac{\beta}{N} H^\pm(x^*, x | a) \right), \end{aligned} \quad (3.4)$$

where

$$\begin{aligned} H^\pm(x^*, x | a) & \equiv H_0^\pm(x^*, x | a) + \gamma H_1^\pm(x^*, x | a) \\ & + h \sum_{k=1}^M x_k^*(a) x_k(a+1) - \frac{hM}{2}, \end{aligned}$$

and

$$\begin{aligned} H_0^\pm(x^*, x | a) & \equiv -\frac{1}{2} \sum_{k=1}^M (x_k^*(a) x_{k+1}(a+1) + x_{k+1}^*(a) x_k(a+1)), \\ H_1^\pm(x^*, x | a) & \equiv -\frac{1}{2} \sum_{k=1}^M (x_{k+1}(a) x_k(a+1) + x_k^*(a) x_{k+1}^*(a+1)). \end{aligned}$$

Inserting (3.3), (3.4) into (3.2), we obtain:

$$\begin{aligned} G_F^\pm Z_F^\pm & = \int dz dz^* \prod_{a=1}^N dx^*(a) dx(a) \exp \left\{ \sum_{k=1}^m z_k^* (z_k + e^\alpha x_k(1)) \right. \\ & + \sum_{k=m+1}^M z_k^* (z_k + x_k(1)) + x^*(1)(x(2) - x(1)) + \dots + x^*(N)(z - x(N)) \\ & \left. - \frac{\beta}{N} (H^\pm(x^*, x | 1) + \dots + H^\pm(x^*, z | N)) \right\}. \end{aligned} \quad (3.5)$$

Let us introduce the notations $x_k(N+1)$ and $x_k^*(0)$ as follows: $x_k(N+1) \equiv z_k$ ($\forall k$), $x_k^*(0) \equiv e^\alpha z_k^*$ (for $1 \leq k \leq m$) or $x_k^*(0) \equiv z_k^*$ (for $m < k \leq M$). Further, we impose the boundary conditions with respect to the counting parameter a :

$$\begin{aligned} x_k(0) & = -e^{-\alpha} x_k(N+1), \quad 1 \leq k \leq m, \\ x_k(0) & = -x_k(N+1), \quad m < k \leq M, \end{aligned}$$

and perform the transition $N \rightarrow \infty$. As a result, the discrete index a varying from 1 to N then becomes a continuous argument $\tau \in [0, \beta]$ (imaginary time; see [26], [19]). The right-hand side of (3.5) then becomes the integral:

$$\int \prod_{\tau \in [0, \beta]} dx^*(\tau) dx(\tau) \exp \left(\int_0^\beta \mathcal{L}(\tau) d\tau \right), \quad (3.6)$$

where $\mathcal{L}(\tau)$ denotes the Lagrangian:

$$\mathcal{L}(\tau) = \sum_{k=1}^M x_k^*(\tau) \frac{dx_k(\tau)}{d\tau} - H^\pm(x^*, x | \tau), \quad (3.7)$$

and the functional variables $x_k(\tau)$ are subjected to the “automorphic” (see (2.11)) conditions:

$$\begin{aligned} x_k(\tau) &= -e^{-\alpha} x_k(\tau + \beta), \quad 1 \leq k \leq m, \\ x_k(\tau) &= -x_k(\tau + \beta), \quad m < k \leq M. \end{aligned} \quad (3.8)$$

Generally speaking, the fields $x_k^*(\tau)$ are independent integration variables. It is convenient to subject $x_k^*(\tau)$ to a requirement analogous to (3.8) but with e^α instead of $e^{-\alpha}$.

The derivation of the representation (3.6)–(3.8) follows [24] strictly, and it does not take into account the peculiar character of our problem: the conditions (3.8) characterize two independent sets of sites. Therefore, the following circumstance becomes essential, which is new in comparison with [24], [27].

It can be assumed that certain representations of the group of shifts of τ by the period β , i.e., $\tau \rightarrow \tau + \beta$, are defined by conventinal (anti-)periodicity rules $x_k(\tau) = \pm x_k(\tau + \beta)$, $k \in \{1, \dots, M\}$, as well as by the conditions (3.8). The action functional of the model, $\int_0^\beta \mathcal{L}(\tau) d\tau$, in the exponent of (3.6) is well-defined provided the Lagrangian $\mathcal{L}(\tau)$ is invariant under the shifts of τ . Such invariance takes place for conventinal boundary conditions provided $\mathcal{L}(\tau)$ is even in powers of the fields.

Let us use (3.8) to calculate the variation $\delta\mathcal{L}(\tau)$ at $m < M$:

$$\begin{aligned} \delta\mathcal{L}(\tau) &\equiv \mathcal{L}(\tau + \beta) - \mathcal{L}(\tau) = \\ &= \frac{1}{2} \left[(e^\alpha - 1) (x_{m+1}^*(\tau) x_m(\tau) + x_M^*(\tau) x_{M+1}(\tau)) \right. \\ &\quad \left. + (e^{-\alpha} - 1) (x_m^*(\tau) x_{m+1}(\tau) + x_{M+1}^*(\tau) x_M(\tau)) \right] \\ &+ \frac{\gamma}{2} \sum_{k=1}^{m-1} \left((e^{2\alpha} - 1) x_{k+1}(\tau) x_k(\tau) + (e^{-2\alpha} - 1) x_k^*(\tau) x_{k+1}^*(\tau) \right) \\ &+ \frac{\gamma}{2} \left[(e^\alpha - 1) (x_{m+1}(\tau) x_m(\tau) + x_{M+1}(\tau) x_M(\tau)) \right. \\ &\quad \left. + (e^{-\alpha} - 1) (x_m^*(\tau) x_{m+1}^*(\tau) + x_M^*(\tau) x_{M+1}^*(\tau)) \right]. \end{aligned}$$

The origin of $\delta\mathcal{L}(\tau)$ is clear: the quadratic forms H_0^\pm are invariant under the replacement

$$x_k \rightarrow \pm e^\alpha x_k, \quad x_k^* \rightarrow \pm e^{-\alpha} x_k^*, \quad (3.9)$$

provided (3.9) is carried out at each site $k \in \{1, \dots, M\}$ (in this case (3.9) looks like a homogeneous “gauge” transformation), and they are not invariant provided (3.9) is valid only for a subset of $\{1, \dots, M\}$ (a nonhomogeneous transformation). However, the forms H_1^\pm are not invariant even for a homogeneous transformation (3.9). The condition (3.8) implies a nonhomogeneous representation of the shifts $\tau \rightarrow \tau + \beta$, and, thus, the invariance turns out to be broken for $\mathcal{L}(\tau)$ (3.7). However, this symmetry can straightforwardly be restored as follows: one should replace $H^\pm(x^*, x \mid \tau)$ in the limiting formula (3.6) by another form $\widetilde{H}^\pm(\tau) \equiv \widetilde{H}^\pm(x^*, x \mid \tau)$ of the following type (we omit the superscript \pm at \widetilde{H}):

$$\widetilde{H}(\tau) = \widetilde{H}_0(\tau) + \gamma \widetilde{H}_1(\tau) + h \sum_{k=1}^M x_k^*(\tau) x_k(\tau) - hM/2, \quad (3.10)$$

where

$$\begin{aligned}
\widetilde{H}_0(\tau) &\equiv -\frac{1}{2} \sum_{k=1}^{M-1} ' \left(x_k^*(\tau) x_{k+1}(\tau) + x_{k+1}^*(\tau) x_k(\tau) \right) \\
&\quad - \frac{1}{2} \left(x_m^*(\tau) x_{m+1}(\tau) e^{\alpha\tau/\beta} + x_{m+1}^*(\tau) x_m(\tau) e^{-\alpha\tau/\beta} \right. \\
&\quad \left. + x_M^*(\tau) x_{M+1}(\tau) e^{-\alpha\tau/\beta} + x_{M+1}^*(\tau) x_M(\tau) e^{\alpha\tau/\beta} \right), \\
\widetilde{H}_1(\tau) &\equiv -\frac{1}{2} \sum_{k=1}^{m-1} \left(x_{k+1}(\tau) x_k(\tau) e^{-2\alpha\tau/\beta} + x_k^*(\tau) x_{k+1}^*(\tau) e^{2\alpha\tau/\beta} \right) \\
&\quad - \frac{1}{2} \sum_{k=m+1}^{M-1} \left(x_{k+1}(\tau) x_k(\tau) + x_k^*(\tau) x_{k+1}^*(\tau) \right) \\
&\quad - \frac{1}{2} \left(x_{m+1}(\tau) x_m(\tau) e^{-\alpha\tau/\beta} + x_m^*(\tau) x_{m+1}^*(\tau) e^{\alpha\tau/\beta} \right. \\
&\quad \left. + x_{M+1}(\tau) x_M(\tau) e^{-\alpha\tau/\beta} + x_M^*(\tau) x_{M+1}^*(\tau) e^{\alpha\tau/\beta} \right),
\end{aligned}$$

where the prime at \sum implies that $k = m$ is skipped in summation. The Lagrangian $\widetilde{\mathcal{L}}(\tau)$ takes the form:

$$\widetilde{\mathcal{L}}(\tau) \equiv \sum_{k=1}^M x_k^*(\tau) \frac{dx_k(\tau)}{d\tau} - \widetilde{H}(x^*, x | \tau). \quad (3.11)$$

Equation (3.11) differs from an expected expression since it contains the exponential factors $\exp(\pm\alpha\tau/\beta)$. The exponentials mentioned ensure periodicity of $\widetilde{\mathcal{L}}(\tau)$ with respect to the imaginary time [23]. Notice that in [24] and [27] the “automorphicity” conditions are the same at each site, and thus the necessity in the “compensating” factors is absent.

The Lagrangian (3.11) is invariant under $\tau \rightarrow \tau + \beta$, the integration measure in (3.6) is also invariant, and, finally, we obtain:

$$G_F^\pm Z_F^\pm = \int \prod_{\tau \in [0, \beta]} dx^*(\tau) dx(\tau) \exp \left(\int_0^\beta \widetilde{\mathcal{L}}(\tau) d\tau \right), \quad (3.12)$$

where $\widetilde{\mathcal{L}}(\tau)$ is given by (3.10), (3.11). For $G_B^\pm Z_B^\pm$ the functional integral representation has the same form (3.12). But because of the presence of the parity operator $(-1)^{\mathcal{N}}$ under the trace symbol in (2.9), we get the corresponding boundary condition in another, in comparison with (3.8), form:

$$\begin{aligned}
x_k(\tau) &= e^{-\alpha} x_k(\tau + \beta), \quad 1 \leq k \leq m, \\
x_k(\tau) &= x_k(\tau + \beta), \quad m < k \leq M
\end{aligned} \quad (3.13)$$

(i.e., two minus are reversed). Substitution of $G_F^\pm Z_F^\pm$, $G_B^\pm Z_B^\pm$, represented by the integrals of the type of (3.12) which are supplied with the appropriate boundary conditions, into (2.9) gives the desired functional integral representation for the generating functional (2.1).

The main statement of the present paper reads that the representations for $G_F^\pm Z_F^\pm$ and $G_B^\pm Z_B^\pm$ given by (3.12) together with the conditions (3.8) and (3.13), respectively, are well-defined relations which lead to correct expressions for the correlation functions.

Actual calculation below is to argue this assertion. We formally consider (3.8) and (3.13) as “automorphic” boundary conditions to distinguish them from more conventional rules known for fermions at $\alpha = i2\pi(k + \frac{1}{2})$ for (3.8), or for bosons at $\alpha = i2\pi k$ for (3.13), $k \in \mathbb{Z}$.

4 Calculation of the functional integrals

In order to proceed with calculation of the integral (3.12), let us pass to the momentum representation:

$$\begin{aligned} x_k(\tau) &= (\beta M)^{-1/2} e^{-i\pi/4} \sum_p e^{i(\omega\tau - i\frac{\alpha}{\beta}\tau + qk)} x_p, \quad 1 \leq k \leq m, \\ x_k(\tau) &= (\beta M)^{-1/2} e^{-i\pi/4} \sum_p e^{i(\omega\tau + qk)} x_p, \quad m < k \leq M, \end{aligned} \quad (4.1)$$

where summation goes over the formal 2-momenta $p = (\omega, q)$: ω implies the Matsubara frequencies $\omega = \pi T(2n + 1)$, $n \in \mathbb{Z}$ (we continue to consider $G_F^\pm Z_F^\pm$), and the quasi-momenta q take their values in the sets X^\pm [11],

$$\begin{aligned} X^+ &= \left\{ q = -\pi + \frac{\pi(2l-1)}{M} \mid l = 1, \dots, M \right\}, \\ X^- &= \left\{ q = -\pi + \frac{2\pi l}{M} \mid l = 1, \dots, M \right\}. \end{aligned} \quad (4.2)$$

Two sets (4.2) are in correspondence with two “spatial” boundary conditions (2.8). As a result of the condition (3.8), the Fermi frequencies in the Fourier expansions for the first m sites are shifted by a purely imaginary number. However, the summation index in (4.1) can obviously taken as ω . We use (4.1) in (3.12) and obtain the following representation:

$$G_F^\pm Z_F^\pm = \int \prod_p dx_p^* dx_p \exp S_F^\pm(\alpha), \quad (4.3)$$

$$\begin{aligned} S_F^\pm(\alpha) &= \frac{\alpha m}{2} + \frac{1}{2} \sum_p (x_p^*, x_{-p}) \begin{pmatrix} i\omega - \varepsilon_q & -\Gamma_q \\ -\Gamma_q & i\omega + \varepsilon_q \end{pmatrix} \begin{pmatrix} x_p \\ x_{-p}^* \end{pmatrix} \\ &+ \frac{\alpha}{2\beta} \sum_{p_1, p_2} (x_{p_1}^*, x_{-p_1}) \begin{pmatrix} \tilde{Q}_{p_1 p_2} & 0 \\ 0 & -\tilde{Q}_{p_1 p_2} \end{pmatrix} \begin{pmatrix} x_{p_2} \\ x_{-p_2}^* \end{pmatrix}, \end{aligned} \quad (4.4)$$

where the notations are defined:

$$\begin{aligned} \varepsilon_q &= h - \cos q, \quad \Gamma_q = \gamma \sin q, \quad \tilde{Q}_{p_1 p_2} = \delta_{\omega_1 \omega_2} Q_{q_1 q_2}, \\ Q_{pq} &= \frac{1}{M} \frac{\sin \frac{m}{2}(p-q)}{\sin \frac{p-q}{2}}. \end{aligned} \quad (4.5)$$

All the quasi-momenta take independently their values in X^+ or X^- . It has to be pointed out that expression $S_F^\pm(\alpha)$ (4.4) should be viewed a bit formally in the case when quasi-momenta belong to the set X^- . Indeed, when $q \in X^-$, the corresponding Fourier coefficients $x_{\omega, q}$ and $x_{\omega, q}^*$ require a separate consideration at $q = 0$ or $q = \pi$. All the

necessary explanations can be found in [42] (see also [11]). We shall assume that when $q = 0$ or $q = \pi$, the corresponding value of the argument $-q$ has to be taken equal also to zero or to π , respectively. Extra term $\alpha m/2$ arises in the matrix representation $S_F^\pm(\alpha)$ (4.4) as a result of an additional assumption about a *fermionic* character of the anti-commutation relations for the coefficients $x_{p_1}^*, x_{p_2}$. Compulsory character of such assumption is due to the fact that the presence of this term plays an important role for obtaining the correct answers for the correlation functions. Calculation for $G_B^\pm Z_B^\pm$ (see (2.9)) is carried out just analogously to that above, but the presence of $(-1)^N$ under the trace symbol results in the boundary conditions (3.13). Eventually, summation in the corresponding quadratic form $S_B^\pm(\alpha)$ goes over the bosonic frequencies $\omega = 2\pi Tn, n \in \mathbb{Z}$, and $G_B^\pm Z_B^\pm$ looks similarly to (4.3), (4.4) provided all the frequencies are replaced.

Using (3.10)–(3.12) at $\gamma = 0$, we obtain the corresponding expression in the XX -case (Eqs.(4.1) are taken without the factors $e^{-i\pi/4}$):

$$\begin{aligned} G_F^\pm Z_F^\pm &= \int \prod_p dx_p^* dx_p \exp(S_F^\pm(\alpha)), \\ S_F^\pm(\alpha) &= \sum_p (i\omega - \varepsilon_q) x_p^* x_p + \frac{\alpha}{\beta} \sum_{p_1, p_2} \tilde{Q}_{p_1 p_2} x_{p_1}^* x_{p_2} + \frac{\beta M h}{2}, \end{aligned} \quad (4.6)$$

where $\varepsilon_q = h - \cos q$ is the band energy of the quasi-particles defined above. When $m = M$, the matrix $Q_{q_1 q_2}$ (4.5) becomes a Kronecker symbol, and therefore $S_F^\pm(\alpha)$ (4.6) is transformed into a free fermionic action with shifted chemical potential.

Let us consider $G_F^+ Z_F^+$, given by (4.3), (4.4), and let us carry out the Bogoliubov transformation in $S_F^+(\alpha)$ with 2×2 matrix \mathbf{g}_θ [42], [11]:

$$(x_p^*, x_{-p}) = (y_p^*, y_{-p}) \mathbf{g}_\theta, \quad (4.7)$$

where

$$\mathbf{g}_\theta \equiv \exp(-i \frac{\theta_q}{2} \sigma^2) \in SU(2), \quad \tan \theta_q = -\frac{\Gamma_q}{\varepsilon_q}, \quad \theta_{-q} = -\theta_q.$$

Here it is assumed that σ^α (α takes values 1, 2, 3) without a lower index implies just a Pauli matrix but not a spin operator on a site. Eventually, we obtain the action

$$\begin{aligned} \tilde{S}_F^\pm(\alpha) &= \frac{\alpha m}{2} + \frac{1}{2} \sum_p (y_p^*, y_{-p}) [i\omega - E_q \sigma^3] \begin{pmatrix} y_p \\ y_{-p}^* \end{pmatrix} \\ &+ \frac{\alpha}{2\beta} \sum_{p_1, p_2} (y_{p_1}^*, y_{-p_1}) \mathbf{g}_{\theta_1} (\tilde{Q}_{p_1 p_2} \sigma^3) \mathbf{g}_{\theta_2}^{-1} \begin{pmatrix} y_{p_2} \\ y_{-p_2}^* \end{pmatrix}, \end{aligned} \quad (4.8)$$

where $\theta_i \equiv \theta_{q_i}$ ($i = 1, 2$), and $E_q \equiv (\varepsilon_q^2 + \Gamma_q^2)^{1/2}$. When $q \in X^-$, the Bogoliubov transformation is carried out by means of (4.7) at $q \neq 0, \pi$, while at $q = 0, \pi$ the remark made after Eq.(4.5) has to be taken into account. The point is that, accordingly to [42], we put at $q = 0, \pi$:

$$y_{\omega,0} = x_{\omega,0}, \quad y_{\omega,0}^* = x_{\omega,0}^*; \quad y_{\omega,\pi} = x_{\omega,\pi}, \quad y_{\omega,\pi}^* = x_{\omega,\pi}^*,$$

and

$$E_0 = h - 1 = \varepsilon_0, \quad E_\pi = h + 1 = \varepsilon_\pi.$$

In both cases, $q \in X^+$ and $q \in X^-$, the final answer is written as a single relation (4.8), where it is assumed that q and $-q$ are understood appropriately.

Substitution of (4.8) into (4.3) (with the change of the integration measure) leads [26] to the answer:

$$G_F^\pm Z_F^\pm = e^{\alpha m/2} \text{Det}^{1/2} A(\alpha), \quad (4.9)$$

$$A_{p_1 p_2}(\alpha) \equiv [i\omega_F - E_{q_1} \sigma^3] \delta_{p_1 p_2} + \frac{\alpha}{\beta} \mathbf{g}_{\theta_1} (\tilde{Q}_{p_1 p_2} \sigma^3) \mathbf{g}_{\theta_2}^{-1}.$$

Calculation for $G_B^\pm Z_B^\pm$ (2.9) is carried out just analogously to that above, and the final answer for $G_B^\pm Z_B^\pm$ looks like (4.9) provided all the frequencies are replaced:

$$G_B^\pm Z_B^\pm = e^{\alpha m/2} \text{Det}^{1/2} \left\{ [i\omega_B - E_{q_1} \sigma^3] \delta_{p_1 p_2} + \frac{\alpha}{\beta} \mathbf{g}_{\theta_1} (\tilde{Q}_{p_1 p_2} \sigma^3) \mathbf{g}_{\theta_2}^{-1} \right\}. \quad (4.10)$$

The partition function of the XY -model is given by (2.10) where Z_F^\pm , Z_B^\pm are given as:

$$Z_F^\pm \equiv \text{Tr} (e^{-\beta H_{XY}^\pm}) = e^{-\beta E_0^\pm} \text{Det} [(i\omega_F - E_q) \delta_{pp'}],$$

$$Z_B^\pm \equiv \text{Tr} ((-1)^N e^{-\beta H_{XY}^\pm}) = e^{-\beta E_0^\pm} \text{Det} [(i\omega_B - E_q) \delta_{pp'}], \quad (4.11)$$

where (see [11])

$$E_0^\pm \equiv -\frac{1}{2} \sum_{q \in X^\pm} E_q, \quad E_q = (\varepsilon_q^2 + \gamma^2 \sin^2 q)^{1/2}.$$

Let use the integral representation (4.6) to obtain the following formal answers in the XX -case [26]:

$$G_F^\pm Z_F^\pm = e^{\beta M h/2} \text{Det} \left[(-i\omega_F + \varepsilon_q) \delta_{pp'} - \frac{\alpha}{\beta} \tilde{Q}_{pp'} \right],$$

$$G_B^\pm Z_B^\pm = e^{\beta M h/2} \text{Det} \left[(-i\omega_B + \varepsilon_q) \delta_{pp'} - \frac{\alpha}{\beta} \tilde{Q}_{pp'} \right], \quad (4.12)$$

and

$$Z_F^\pm = e^{\beta M h/2} \text{Det} [(i\omega_F - \varepsilon_q) \delta_{pp'}],$$

$$Z_B^\pm = e^{\beta M h/2} \text{Det} [(i\omega_B - \varepsilon_q) \delta_{pp'}]. \quad (4.13)$$

In Eqs.(4.9)–(4.13) we use the notations ω_F and ω_B to stress the character, e.g., fermionic or bosonic, of the corresponding frequencies. The symbol ‘Det’ denotes determinants of infinite-dimensional matrices, while ‘det’ is reserved for conventional matrices. Derivations of the representations (4.12) for $G_F^\pm Z_F^\pm$ and $G_B^\pm Z_B^\pm$, as well as of (4.13) for Z_F^\pm and Z_B^\pm , are carried out analogously. It is convenient to denote the matrix operators, which appear in (4.9), (4.10), (4.12), as $A(\alpha) \equiv A_\alpha$, while those in (4.11), (4.13) – as A .

5 Zeta-regularization (Zeta-functions in the series form)

We shall use ζ -regularization [39] in order to assign meaning to the determinants in (4.9)–(4.13). We shall begin with the introductory notes. Usually, a generalized ζ -function is related to an elliptic operator. Precisely, let \mathcal{A} be a non-negative elliptic operator of

order $p > 0$ on a compact d -dimensional smooth manifold. Let its eigen-values λ_n being enumerated by the multi-index n . The series

$$\zeta(s | \mathcal{A}) = \sum_{\lambda_n \neq 0} (\lambda_n)^{-s}, \quad (5.1)$$

which is convergent at $\Re s > d/p$, defines the generalized ζ -function of the operator \mathcal{A} , $\zeta(s | \mathcal{A})$. This series defines $\zeta(s | \mathcal{A})$ as the meromorphic function of the variable $s \in \mathcal{T}$, which can be analytically continued to $s = 0$. The formal relation

$$\lim_{s \rightarrow 0} \frac{d\zeta}{ds}(s | \mathcal{A}) = \lim_{s \rightarrow 0} \left[- \sum_{\lambda_n \neq 0} \frac{\log \lambda_n}{(\lambda_n)^s} \right] = - \log \left(\prod_{\lambda_n \neq 0} \lambda_n \right)$$

allows to define a regularized determinant of \mathcal{A} as follows:

$$\log \text{Det } \mathcal{A} = - \lim_{s \rightarrow 0} \frac{d}{ds} \zeta(s | \mathcal{A}) \quad (5.2)$$

The Riemann ζ -function,

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s}, \quad \Re s > 1, \quad (5.3)$$

and the generalized ζ -function,

$$\zeta(s, \alpha) = \sum_{n=0}^{\infty} (n + \alpha)^{-s}, \quad \alpha \neq 0, -1, -2, \dots, \quad (5.4)$$

are meromorphic in s , have a simple pole at $s = 1$ with residue 1, and possess a continuation at $s = 0$ [46] (see also [47]). These functions can formally be considered as particular cases of the series (5.1). Notice that $\zeta(s, \frac{1}{2})$ is the Gurvitz ζ -function [46], and $\zeta(s, 1) = \zeta(s)$.

Starting with (5.1), one can represent $\zeta(s | \mathcal{A})$ as a Mellin transform:

$$\zeta(s | \mathcal{A}) = \frac{1}{\Gamma(s)} \int_0^{\infty} t^{s-1} [\text{Tr}(e^{-\mathcal{A}t}) - \dim(\ker \mathcal{A})] dt. \quad (5.5)$$

The integral (5.5) is defined at sufficiently large positive $\Re s$ (precisely, at $\Re s > d/p$); for other $\Re s$ its analytic continuation is required. Equation (5.5) can be related [38], [39] to the definition of $\text{Det } \mathcal{A}$ by means of the proper time regularization [48], [49]:

$$\log \frac{\text{Det } \mathcal{A}}{\text{Det } \mathcal{A}_0} = \text{Tr} \left[\int_0^{\infty} (e^{-\mathcal{A}_0 t} - e^{-\mathcal{A} t}) \frac{dt}{t} \right]. \quad (5.6)$$

The definitions of $\log \text{Det } \mathcal{A}$ by means of (5.2), (5.5), and by means of (5.6) coincide up to an infinite additive constant.

Now one can pass to calculation of the determinants (4.11). Let us define the following series, which can be expressed through $\zeta(s, \alpha)$ (5.4):

$$\begin{aligned} \zeta_F^{\pm}(s | A) &\equiv \sum_{\omega_F, q \in X^{\pm}} (i\omega_F - E_q)^{-s} \\ &= \left(\frac{\beta}{2\pi i} \right)^s \sum_{q \in X^{\pm}} \left[\zeta \left(s, \frac{1}{2} + i \frac{\beta E_q}{2\pi} \right) + (-1)^s \zeta \left(s, \frac{1}{2} - i \frac{\beta E_q}{2\pi} \right) \right], \end{aligned} \quad (5.7)$$

$$\begin{aligned}
\zeta_B^\pm(s | A) &\equiv \sum_{\omega_B, q \in X^\pm} (i\omega_B - E_q)^{-s} \\
&= \left(\frac{\beta}{2\pi i}\right)^s \sum_{q \in X^\pm} \left[\zeta\left(s, i\frac{\beta E_q}{2\pi}\right) + (-1)^s \zeta\left(s, -i\frac{\beta E_q}{2\pi}\right) \right] - \sum_{q \in X^\pm} (-E_q)^{-s}.
\end{aligned} \tag{5.8}$$

The series $\zeta_F^\pm(s | A)$ and $\zeta_B^\pm(s | A)$ should be considered as the generalized ζ -functions of the diagonal operators A (see (4.11), (4.13)) in the series form (5.1). The analytic continuations for $\zeta(s, z)$ are known [46]:

$$\zeta(0, z) = \frac{1}{2} - z, \quad \zeta'(0, z) = \log \frac{\Gamma(z)}{(2\pi)^{1/2}}, \tag{5.9}$$

and they lead to the following answers:

$$\begin{aligned}
-\lim_{s \rightarrow 0} \frac{d}{ds} \zeta_F^\pm(s | A) &= \sum_{q \in X^\pm} \log(1 + e^{c\beta E_q}), \\
-\lim_{s \rightarrow 0} \frac{d}{ds} \zeta_B^\pm(s | A) &= \sum_{q \in X^\pm} \log(1 - e^{c\beta E_q}),
\end{aligned} \tag{5.10}$$

where $c = \pm 1$ due to an arbitrariness when differentiating $(-1)^s = \exp(\pm i\pi s)$.

Choosing $c = -1$, and combining (5.10) with (5.2), one obtains the following relations of the XY -model [10], [11]:

$$\begin{aligned}
Z_F^\pm &= e^{-\beta E_0^\pm} \prod_{q \in X^\pm} (1 + e^{-\beta E_q}) = \prod_{q \in X^\pm} 2 \cosh \frac{\beta E_q}{2}, \\
Z_B^\pm &= e^{-\beta E_0^\pm} \prod_{q \in X^\pm} (1 - e^{-\beta E_q}) = \prod_{q \in X^\pm} 2 \sinh \frac{\beta E_q}{2}.
\end{aligned} \tag{5.11}$$

The total partition function should be calculated accordingly to (2.10), the free energy is $F = -(1/\beta M) \log Z$, while arbitrariness in the choice of c does not influence the magnetization $M_z = -\partial F / \partial h$ and the entropy $S = -\partial F / \partial T$. Specifically, one gets in the thermodynamic limit [10]:

$$F = -\frac{1}{2\pi\beta} \int_0^\pi \log(2(1 + \cosh \beta E_q)) dq. \tag{5.12}$$

All the formulas obtained can be reduced at $\gamma \rightarrow 0$ to those of the XX -model.

6 Determinants of the operators $A(\alpha)$

6.1 The regularization (Zeta-functions in the integral form)

Thus, in the previous section we have defined ζ -functions of the diagonal operators A given by (4.11), (4.13) in the series form. Let us now use (5.5) to calculate the regularized determinants of the non-diagonal operators A_α given by (4.9), (4.10), (4.12). For instance, let us now proceed with the calculation of G_F^\pm (4.12).

Let us begin with the formal integral

$$\frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \text{Tr} \left[e^{(i\omega_F - \widehat{\varepsilon} + \frac{\alpha}{\beta} \widehat{Q})t} \right] dt, \quad (6.1)$$

where $\widehat{\varepsilon}$ and \widehat{Q} imply the matrices in the momentum space, $\text{diag} \{\varepsilon_q\}$ and Q_{pq} (4.5), accordingly, while the indices p, q run independently over X^+ or X^- . Trace ‘Tr’ in (6.1) is considered as a matrix one over the corresponding 2-momenta $p = (\omega, q)$ which label entries of our matrix operators. Convergence of the integral (6.1) at the upper bound is respected at sufficiently large $h > h_c = 1$ (h_c is the critical magnetic field [4]). Regularization of the integral is necessary at the lower bound.

Let us use the asymptotical relation

$$\text{Tr} \left[e^{(i\omega_F - \widehat{\varepsilon} + \frac{\alpha}{\beta} \widehat{Q})t} \right] \xrightarrow{t \rightarrow 0} \phi_0,$$

where ϕ_0 is an infinite constant equal to $\text{Tr}(\delta_{pp'}) \equiv \sum_{\omega_F} \text{tr} \widehat{\delta}$ ($\widehat{\delta}$ is a unit $M \times M$ matrix).

Let us define the function $\rho(t)$:

$$\rho(t) \equiv \text{Tr} \left[e^{(i\omega_F - \widehat{\varepsilon} + \frac{\alpha}{\beta} \widehat{Q})t} \right] - \phi_0, \quad 0 \leq t < 1, \quad (6.2)$$

and divide the integral (6.1) into two parts. We rewrite (6.1) using (6.2) as follows:

$$\frac{1}{\Gamma(s)} \int_1^\infty t^{s-1} \text{Tr} \left[e^{(i\omega_F - \widehat{\varepsilon} + \frac{\alpha}{\beta} \widehat{Q})t} \right] dt + \frac{1}{\Gamma(s)} \int_0^1 t^{s-1} \rho(t) dt + \frac{\phi_0}{s\Gamma(s)}. \quad (6.3)$$

The function $\rho(t)$ is a formal series in powers of t^n , $n \geq 1$. Besides,

$$\frac{1}{s\Gamma(s)} \simeq 1 + \gamma s + o(s), \quad \gamma = -\psi(1), \quad (6.4)$$

where $\psi(z) = (d/dz) \log \Gamma(z)$. Therefore, (6.3), which is regular at $s \rightarrow 0$, defines an analytic continuation of (6.1) at any $\Re s \geq 0$. It just can be considered as the definition of $\zeta_F^\pm(s | A_\alpha)$ in the right half-plane of $\mathcal{C} \ni s$.

Let us now consider the constant ϕ_0 and the coefficients which define $\rho(t)$. In our situation all these coefficients are given by divergent series, but finite (i.e., regularized) values can be assigned to them by means of reductions of the series to zeta-functions (5.3), (5.4), i.e., to their particular values at special arguments [46].

First of all, using $\zeta(0) = -\frac{1}{2}$ one obtains:

$$\phi_0 = M \sum_{\mathbb{Z}} 1 = M(2\zeta(0) + 1) = 0,$$

where we can equivalently replace $\sum_{\mathbb{Z}}$ and $2\zeta(0) + 1$ by $\sum_{\mathbb{Z} + \frac{1}{2}}$ and $2\zeta\left(0, \frac{1}{2}\right)$, respectively

(“ ζ -regularized measure” of the set \mathbb{Z} is zero). Further, the divergence of the coefficients at the powers of t in $\rho(t)$ is given by the divergent sums $\sum_{n \in \mathbb{Z} + \frac{1}{2}} n^m$. It is reasonable to

consider such sums as zeros at $m = 2k + 1$, $k \in \mathbb{Z}^+$, since $n^m \equiv \left(l + \frac{1}{2}\right)^m$ are odd. If $m = 2k$, $k \in \mathbb{Z}^+$, then

$$\sum_{n \in \mathbb{Z} + \frac{1}{2}} n^m = 2 \sum_{l=0}^{\infty} \left(l + \frac{1}{2}\right)^m = 2\zeta\left(-2k, \frac{1}{2}\right) = 2\left(\frac{1}{2^{2k}} - 1\right)\zeta(-2k).$$

But $\zeta(-2k) = 0$ at $k \geq 1$. It can be concluded that all “ ζ -regularized” coefficients are zero for $\rho(t)$, corresponding to our A_α , and, thus, only the first term is relevant in (6.3).

Let use (6.4) to pass from (6.3) to the relation:

$$-\lim_{s \rightarrow 0} \frac{d}{ds} \zeta_F^\pm(s | A_\alpha) = - \int_1^\infty \text{tr} \left[e^{(-\widehat{\varepsilon} + \frac{\alpha}{\beta} \widehat{Q})t} \right] \left(\sum_{\omega_F} e^{i\omega_F t} \right) \frac{dt}{t} - \int_0^1 \rho(t) \frac{dt}{t} - \gamma \phi_0, \quad (6.5)$$

where the Poisson summation formula enables to sum up over ω_F . Then, R.H.S. of (6.5) takes the form:

$$\begin{aligned} & -\text{tr} \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \left(e^{-\beta \widehat{\varepsilon} + \alpha \widehat{Q}} \right)^k - \int_0^1 \rho(t) \frac{dt}{t} - \gamma \phi_0 \\ & = \log \det \left(\widehat{\delta} + e^{-\beta \widehat{\varepsilon} + \alpha \widehat{Q}} \right) - \int_0^1 \rho(t) \frac{dt}{t} - \gamma \phi_0, \end{aligned}$$

where $\widehat{\delta}$ is a unit $M \times M$ matrix. Let us also take into account that $\widehat{Q}^2 = \widehat{Q}$, and so, $e^{\alpha \widehat{Q}} - \widehat{\delta} = (e^\alpha - 1)\widehat{Q}$. Therefore,

$$G_F^\pm = \frac{\text{Det} \left[(i\omega_F - \varepsilon_q) \delta_{pp'} + \frac{\alpha}{\beta} \widetilde{Q}_{pp'} \right]}{\text{Det} [(i\omega_F - \varepsilon_q) \delta_{pp'}]} = \det \left[\widehat{\delta} + (e^\alpha - 1)\widehat{Q}(\widehat{\delta} + e^{\beta \widehat{\varepsilon}})^{-1} \right]. \quad (6.6)$$

Additional renormalization of $\rho(t)$ and ϕ_0 (to zero, in fact) is irrelevant for G_F^\pm written as the ratio of the determinants. However, when $m = M$, the corresponding operator A_α becomes diagonal since \widehat{Q} becomes a unit matrix $\widehat{\delta}$. In this case, we can use ζ -function in the series form (5.1). Transparent adjusting of (5.7)–(5.10) for this case (i.e., for $m = M$) gives the same answer as that given by (6.5) where $\rho(t)$ and ϕ_0 are taken zero. Further, we proceed similarly to obtain:

$$G_B^\pm = \det \left[\widehat{\delta} + \widehat{M}_B(\alpha) \right], \quad (6.7a)$$

where we introduced the matrix notation

$$\widehat{M}_{F,B}(\alpha) \equiv \frac{(e^\alpha - 1)\widehat{Q}}{\widehat{\delta} \pm \exp(\beta \widehat{\varepsilon})}. \quad (6.7b)$$

The matrices $\widehat{M}_{F,B}(\alpha)$ are of the size $M \times M$; we take $+$ or $-$ in the R.H.S. of (6.7b) provided the subscript in the L.H.S. is F or B , respectively.

In deriving (6.6), (6.7), we have restricted ourselves to the case where $h > 1$. For $0 < h < 1$, the energy ε_q is not strictly positive, and a potential problem of convergency of the integral (6.1) at the upper bound arises. It can be shown that in this case it is necessary to use the integral representation (6.1) to calculate a regularized value of $\text{Det}^{1/2}(A_\alpha A_\alpha^*)$,

where A_α^* is a complex conjugated to A_α . Consideration of the corresponding complex “phase” of the determinant of A_α leads to the same final answer as that at $h > 1$.

Let us illustrate the last statements by the following calculation. We are going to calculate $\text{Det}(i\omega_F + \lambda)$. First of all, let us use (5.5) to calculate

$$\text{Det}^{1/2}(\omega_F^2 + \lambda^2) = \sqrt{\text{Det}(i\omega_F + \lambda) \text{Det}(-i\omega_F + \lambda)},$$

where λ is nonzero real number. Let us start with the representation

$$\frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \text{Tr} \left[e^{-(\omega_F^2 + \lambda^2)t} \right] dt.$$

We use the estimation:

$$\text{Tr} \left[e^{-(\omega_F^2 + \lambda^2)t} \right] \underset{t \rightarrow 0}{\sim} \frac{\beta}{2(\pi t)^{1/2}},$$

where the Poisson summation formula is used to re-express the series

$$\sum_{\omega_F} \exp(-\omega_F^2 t) = \frac{\beta}{2\sqrt{\pi t}} \sum_{\mathbb{Z}} (-1)^k \exp\left(-\frac{\beta^2 k^2}{4t}\right), \quad 0 \leq t < 1,$$

and we define the function $\rho(t)$ (compare with (6.2)) as follows:

$$\rho(t) \equiv \text{Tr} \left[e^{-(\omega_F^2 + \lambda^2)t} \right] - \frac{\beta}{2(\pi t)^{1/2}}.$$

Now, the corresponding generalized ζ -function of the diagonal matrix operator $\text{diag} \{\omega_F^2 + \lambda^2\}$ takes the form:

$$\begin{aligned} \zeta(s | \text{diag} \{\omega_F^2 + \lambda^2\}) &\equiv \frac{1}{\Gamma(s)} \left[\int_1^\infty t^{s-1} \text{Tr} \left(e^{-(\omega_F^2 + \lambda^2)t} \right) dt \right. \\ &\quad \left. + \int_0^1 t^{s-1} \rho(t) dt + \frac{\beta}{2\pi^{1/2}} (s - 1/2)^{-1} \right]. \end{aligned} \quad (6.8)$$

Equation (6.8) defines an analytic continuation of ζ -function in the right half-plane of $\mathcal{C} \ni s$.

Using (6.8) we proceed with the calculation of the logarithm of the determinant $\text{Det}^{1/2}(\omega_F^2 + \lambda^2)$:

$$\begin{aligned} -\frac{1}{2} \lim_{s \rightarrow 0} \frac{d}{ds} \zeta(s | \text{diag} \{\omega_F^2 + \lambda^2\}) &= -\frac{1}{2} \int_1^\infty \left(\sum_{\omega_F} e^{-\omega_F^2 t} \right) e^{-\lambda^2 t} \frac{dt}{t} - \frac{1}{2} \int_0^1 \rho(t) \frac{dt}{t} + \frac{\beta}{2\pi^{1/2}} \\ &= \log(1 + e^{-\beta|\lambda|}) - \frac{\beta}{4\pi^{1/2}} \left(\int_1^\infty e^{-\lambda^2 t} \frac{dt}{t^{3/2}} + \int_0^1 (e^{-\lambda^2 t} - 1) \frac{dt}{t^{3/2}} \right) + \frac{\beta}{2\pi^{1/2}} \\ &= \log\left(2 \text{ch} \frac{\beta|\lambda|}{2}\right). \end{aligned} \quad (6.9)$$

In right-hand side of (6.9) we can replace $|\lambda|$ by λ . Thus we have obtained the regularized value for the logarithm of $\text{Det}^{1/2}(\omega_F^2 + \lambda^2)$. We determine the “phase” of $\text{Det}(i\omega_F + \lambda)$ as follows:

$$\sum_{\omega_F} \arctan \frac{\omega_F}{\lambda} = \frac{-i}{2} \sum_{\omega_F} \log \frac{\lambda + i\omega_F}{\lambda - i\omega_F} = -ic \frac{\beta\lambda}{2}, \quad c = \pm 1, \quad (6.10)$$

where we take into account the fact that $\sum_{\mathbb{Z}} 1 = 2\zeta(0) + 1 = 0$, and we use

$$-\lim_{s \rightarrow 0} \frac{d}{ds} \left(\sum_{\omega_F} (i\omega_F + \ell)^{-s} \right) = \log(1 + e^{-c\beta\ell})$$

at $\ell = \pm\lambda$. Combining (6.9) and (6.10), we obtain, in agreement with the previous calculations (5.7)–(5.10), the following answer:

$$\text{Det}(i\omega_F + \lambda) = 1 + e^{c\beta\lambda}. \quad (6.11)$$

Therefore, for any sign of the parameter (“energy”) λ , we can use a freedom in the choice of c so that the final result, say, for the eigen-value matrix $\hat{\varepsilon} = \text{diag} \{\varepsilon_q\}$ with ε_q (4.5) will be the same at $0 < h < 1$ as that for the magnetic field $h > 1$. Since our matrix operators are diagonalizables, the calculation of (6.11) by means of (6.8)–(6.10) justifies our manipulations leading to (6.6), (6.7) at any $h > 0$. For the bosonic frequencies ω_B the situation is similiar.

Now, let us turn to the XY -case. We shall define the regularized determinant of the matrix operator $A(\alpha)$ (4.9) by means of the generalized zeta-function of this operator $\zeta(s|A(\alpha))$ as follows:

$$\log \text{Det}^{1/2} A(\alpha) = -\frac{1}{2} \lim_{s \rightarrow 0} \frac{d}{ds} \zeta(s|A(\alpha)),$$

where a standard representation of $\zeta(s|A(\alpha))$ by the Mellin integral (5.5) is meant. Referring to the previous calculations concerning the XX -case, we shall write the answers as follows:

$$\begin{aligned} G_F^\pm &= e^{\alpha m/2} \frac{\text{Det}^{1/2} \left[i\omega_F - \hat{E} \otimes \sigma^3 + \frac{\alpha}{\beta} \tilde{g} (\hat{Q} \otimes \sigma^3) \tilde{g}^{-1} \right]}{\text{Det}^{1/2} [i\omega_F - \hat{E} \otimes \sigma^3]} \\ &= \det_M^{1/2} (e^{\alpha \hat{Q}}) \det_{2M}^{1/2} \left\{ \tilde{I} + \frac{\tilde{g} [\hat{Q} \otimes (\exp(-\alpha \sigma^3) - I)] \tilde{g}^{-1}}{\tilde{I} + \exp(-\beta \hat{E} \otimes \sigma^3)} \right\}, \end{aligned} \quad (6.12)$$

$$Z_F^\pm = \det_{2M}^{1/2} \left\{ \tilde{I} + \exp(\beta \hat{E} \otimes \sigma^3) \right\}. \quad (6.13)$$

The determinants of the infinite-dimensional and finite-dimensional matrices are denoted in (6.12), (6.13) as ‘Det’ and ‘det’, respectively, while the indices M and $2M$ imply the size of the matrices. In (6.12), \tilde{I} denotes a unit $2M \times 2M$ matrix, \tilde{g} denotes a block-diagonal $2M \times 2M$ matrix with the blocks on its principal diagonal given by the matrices \mathbf{g}_θ defined in (4.7); \hat{Q} and \hat{E} are $M \times M$ matrices with the entries $Q_{q_1 q_2}$ and $E_{q_1} \delta_{q_1 q_2}$, correspondingly, and I is 2×2 unit matrix. Besides, the following relations are used:

$$\exp(-\alpha \tilde{g} (\hat{Q} \otimes \sigma^3) \tilde{g}^{-1}) - \tilde{I} = \tilde{g} [\hat{Q} \otimes (\exp(-\alpha \sigma^3) - I)] \tilde{g}^{-1},$$

and $\det(\exp \alpha \hat{Q}) = \exp(\alpha m)$ (see notations in (4.5)). The notations for tensor products in (6.12), (6.13) are in agreement with the matrix notations in (4.8)–(4.10).

Let us verify some reductions of the relations (6.12), (6.13). First of all, let us calculate Z_F^\pm (6.13):

$$Z_F^\pm = \sqrt{\prod_{q \in X^\pm} (1 + e^{\beta E_q})(1 + e^{-\beta E_q})} = \prod_{q \in X^\pm} 2 \cosh \frac{\beta E_q}{2}. \quad (6.14)$$

Further, we shall consider (6.12). When $m = M$, the matrix \hat{Q} becomes a unit matrix $\hat{\delta}$, and we obtain at $\alpha = i\pi$ (see (5.11), as well as the definitions (2.9) and (2.10)):

$$G_F^\pm = \prod_{q \in X^\pm} \tanh \frac{\beta E_q}{2} = Z_B^\pm / Z_F^\pm \quad (6.15)$$

Let us now put $m = M$, and α is arbitrary. Then, we obtain from (6.12):

$$\begin{aligned} G_F^\pm &= e^{\alpha M/2} \sqrt{\prod_{q \in X^\pm} \det_2 \left[I - \frac{(1 - \operatorname{ch} \alpha)I + \operatorname{sh} \alpha \mathbf{g}_{2\theta} \sigma^3}{I + \exp(-\beta E_q \sigma^3)} \right]} \\ &= e^{\alpha M/2} \sqrt{\prod_{q \in X^\pm} \left(\operatorname{ch}^2 \frac{\alpha}{2} - \operatorname{sh} \alpha \cos \theta_q \operatorname{th} \frac{\beta E_q}{2} + \operatorname{sh}^2 \frac{\alpha}{2} \operatorname{th}^2 \frac{\beta E_q}{2} \right)}, \end{aligned} \quad (6.16)$$

where $\mathbf{g}_{2\theta}$ is the matrix of rotation by the angle $2\theta_q$, I is a 2×2 unit matrix. On the other hand, the result of [11] reads:

$$G_F^\pm = \det_M \left(\hat{\delta} + \widehat{K}_F(\alpha) \right), \quad \widehat{K}_F(\alpha) \equiv (e^\alpha - 1) \frac{\hat{Q}}{2} \operatorname{diag} \left\{ 1 - e^{i\theta_q \operatorname{th} \frac{\beta E_q}{2}} \right\}. \quad (6.17)$$

Direct calculations of G_F^\pm by means of (6.17) taken at $m = M$, and by means of (6.16), coincide. Finally, let us take $\gamma = 0$ while α and m both are arbitrary in (6.12). Then we obtain the answer (6.6) for the XX -case as follows:

$$\begin{aligned} G_F^\pm &= \det_{2M}^{1/2} \begin{pmatrix} \exp(\alpha \hat{Q}) & 0 \\ 0 & \hat{\delta} \end{pmatrix} \det_{2M}^{1/2} \begin{pmatrix} \hat{\delta} + \frac{\exp(-\alpha \hat{Q}) - \hat{\delta}}{\hat{\delta} + \exp(-\beta \hat{\varepsilon})} & 0 \\ 0 & \hat{\delta} + \frac{\exp(\alpha \hat{Q}) - \hat{\delta}}{\hat{\delta} + \exp(\beta \hat{\varepsilon})} \end{pmatrix} \\ &= \det_M \left(\hat{\delta} + \frac{\exp(\alpha \hat{Q}) - \hat{\delta}}{\hat{\delta} + \exp(\beta \hat{\varepsilon})} \right), \end{aligned} \quad (6.18)$$

where the matrices \hat{Q} and $\hat{\delta}$ are defined above, and $\hat{\varepsilon} = \operatorname{diag} \{ \varepsilon_q \}$, $\varepsilon_q \equiv h - \cos q$.

It is clear from (6.14)–(6.16), (6.18) that the representations (6.12), (6.13) are in agreement with the results (6.6), (6.7) [23], and they reproduce the relations of the XX model [4], [10], [11], correctly. Calculation for $G_B^\pm Z_B^\pm$ is carried out just analogously to that above. The final answers for G_B^\pm and Z_B^\pm are:

$$G_B^\pm = e^{\alpha m/2} \frac{\operatorname{Det}^{1/2} \left[i\omega_B - \hat{E} \otimes \sigma^3 + \frac{\alpha}{\beta} \tilde{g}(\hat{Q} \otimes \sigma^3) \tilde{g}^{-1} \right]}{\operatorname{Det}^{1/2} [i\omega_B - \hat{E} \otimes \sigma^3]}$$

$$= \det_M^{1/2}(e^{\alpha\hat{Q}}) \det_{2M}^{1/2} \left\{ \tilde{I} + \tilde{M}_B(\alpha) \right\}, \quad (6.19a)$$

$$Z_F^\pm = \det_{2M}^{1/2} \left\{ \tilde{I} - \exp(\beta\hat{E} \otimes \sigma^3) \right\}, \quad (6.19b)$$

where

$$\tilde{M}_{F,B}(\alpha) \equiv \frac{\tilde{g}[\hat{Q} \otimes (\exp(-\alpha\sigma^3) - I)]\tilde{g}^{-1}}{\tilde{I} \pm \exp(-\beta\hat{E} \otimes \sigma^3)}. \quad (6.19c)$$

In (6.19c) it is also meant that $+$ or $-$ correspond to F or B , accordingly. We see that the answers (6.12) and (6.19a) differ only with respect to the signs at $\exp(\pm\beta\hat{E} \otimes \sigma^3)$. Analogously, the results in [11] for G_F^\pm and G_B^\pm also differ only with respect to the signs in front of $\exp(\beta E_q)$.

It is appropriate to notice that the representation

$$\begin{aligned} G_F^\pm &= e^{\alpha m/2} \text{Det}^{1/2} \left\{ \tilde{I} + \frac{\alpha}{\beta} \frac{\tilde{g}(\hat{Q} \otimes \sigma^3) \tilde{g}^{-1}}{i\omega_F - \hat{E} \otimes \sigma^3} \right\} \\ &= e^{\alpha m/2} \exp \left\{ \frac{1}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \text{Tr} \left[\frac{\alpha}{\beta} \frac{\tilde{g}(\hat{Q} \otimes \sigma^3) \tilde{g}^{-1}}{i\omega_F - \hat{E} \otimes \sigma^3} \right]^k \right\} \end{aligned} \quad (6.20)$$

(which implies regularization of $\text{Det} A(\alpha)$ more conventional for quantum field theory) leads to the same numerical coefficients at the powers of α , as Eq.(6.12). For the XX -case, (6.20) acquires the following form:

$$G_F^\pm = \text{Det} \left\{ \hat{\delta} + \frac{\alpha}{\beta} \frac{\hat{Q}}{i\omega_F - \hat{\varepsilon}_q} \right\} = \exp \left\{ \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \text{Tr} \left[\frac{\alpha}{\beta} \frac{\hat{Q}}{i\omega_F - \hat{\varepsilon}_q} \right]^k \right\} \quad (6.21)$$

In (6.20) and (6.21), \tilde{I} and $\hat{\delta}$ imply the corresponding unit operators.

6.2 Differentiation of the determinants

Calculation of the correlation functions by means of the generating functional $G(\alpha, m)$ (2.1) is related with differentiations of it over α and m [1], [3], [4], [7], [9], [10], [11], [15]. In fact, in order to calculate correlators of z -components of spins (the operator of third component of spin, σ_m^z , is defined as σ^z at m th site), we differentiate $G(\alpha, m)$ over α at $\alpha = 0$ as follows [1], [4]:

$$\langle Q^n(m) \rangle = \lim_{\alpha \rightarrow 0} \frac{d^n}{d\alpha^n} G(\alpha, m). \quad (6.22)$$

However, with regard at (6.1), it is suffice to do only a first differentiation. The other ones occur as usual differentiations of matrices [50].

The operators in question, $A(\alpha)$, are linear in α : $A(\alpha) \equiv A_1 + \alpha A_2$. Let us calculate the first derivative of $\text{Det} A(\alpha)$ using the formal integral (6.1):

$$\frac{(d/d\alpha)\text{Det} A(\alpha)}{\text{Det} A(\alpha)} = -\frac{d}{d\alpha} \left(\int_0^\infty \text{Tr} (e^{A(\alpha)t}) \frac{dt}{t} \right) \quad (6.23)$$

(the regularization at $t \searrow 0$ is irrelevant for the differentiation over the parameter). In the spirit of the Ray–Singer–Schwarz lemma [51], we shall use in (6.23) the following relation:

$$\frac{d}{d\alpha} \left(\text{Tr} (e^{A(\alpha)t}) \right) = t \frac{d}{dt} \text{Tr} (B(\alpha) e^{A(\alpha)t}), \quad B(\alpha) \equiv A_2 A^{-1}(\alpha).$$

Then, the integral over t can be calculated, and we obtains in the XX -case:

$$\begin{aligned} \frac{d}{d\alpha} (\log \text{Det } A_\alpha) &= \text{Tr } B_\alpha \\ &= \text{Tr} \left(\frac{\hat{Q}}{\beta} (i\omega_F - \hat{\varepsilon} + \frac{\alpha}{\beta} \hat{Q})^{-1} \right) = \text{tr} \left(\hat{Q} (1 + e^{\beta \hat{\varepsilon} - \alpha \hat{Q}})^{-1} \right), \end{aligned} \quad (6.24)$$

where the ‘fermionic’ A_α (4.12) is meant, and the Cauchy formula for matrices [50] is used to sum up over the frequencies. In the XY -case, for the matrix operator, say, A_α (4.9), the answer reads:

$$\frac{d}{d\alpha} (\log \text{Det}^{1/2} A_\alpha) = -\frac{1}{2} \text{tr} \left(\frac{\tilde{g} (\hat{Q} \otimes \sigma^3) \tilde{g}^{-1}}{\tilde{I} + \exp(-\beta \hat{E} \otimes \sigma^3 + \alpha \tilde{g} (\hat{Q} \otimes \sigma^3) \tilde{g}^{-1})} \right). \quad (6.25)$$

Knowing (6.24), (6.25), one can carry out all the differentiations required. Thus, we obtain,

a) in the XX -case:

$$\lim_{\alpha \rightarrow 0} \frac{(d/d\alpha) \text{Det } A_\alpha}{\text{Det } A_\alpha} = \text{tr} \left(\hat{Q} (\hat{\delta} + e^{\beta \hat{\varepsilon}})^{-1} \right), \quad (6.26)$$

$$\lim_{\alpha \rightarrow 0} \frac{(d^2/d\alpha^2) \text{Det } A_\alpha}{\text{Det } A_\alpha} = \text{tr} \left(\hat{Q} (\hat{\delta} + e^{\beta \hat{\varepsilon}})^{-1} \right) +$$

$$+ \text{tr}^2 \left(\hat{Q} (\hat{\delta} + e^{\beta \hat{\varepsilon}})^{-1} \right) - \text{tr} \left(\hat{Q} (\hat{\delta} + e^{\beta \hat{\varepsilon}})^{-1} \hat{Q} (\hat{\delta} + e^{\beta \hat{\varepsilon}})^{-1} \right),$$

etc.;

b) in the XY -case:

$$\lim_{\alpha \rightarrow 0} \frac{(d/d\alpha) \text{Det}^{1/2} A_\alpha}{\text{Det}^{1/2} A_\alpha} = -\frac{1}{2} \text{tr} \left(\frac{\tilde{g} (\hat{Q} \otimes \sigma^3) \tilde{g}^{-1}}{\tilde{I} + \exp(-\beta \hat{E} \otimes \sigma^3)} \right), \quad (6.27)$$

$$\lim_{\alpha \rightarrow 0} \frac{(d^2/d\alpha^2) \text{Det}^{1/2} A_\alpha}{\text{Det}^{1/2} A_\alpha} = \frac{1}{2} \text{tr} \left(\frac{\tilde{g} (\hat{Q} \otimes I) \tilde{g}^{-1}}{\tilde{I} + \exp(-\beta \hat{E} \otimes \sigma^3)} \right)$$

$$+ \frac{1}{4} \text{tr}^2 \left(\frac{\tilde{g} (\hat{Q} \otimes \sigma^3) \tilde{g}^{-1}}{\tilde{I} + \exp(-\beta \hat{E} \otimes \sigma^3)} \right) - \frac{1}{2} \text{tr} \left(\frac{\tilde{g} (\hat{Q} \otimes \sigma^3) \tilde{g}^{-1}}{\tilde{I} + \exp(-\beta \hat{E} \otimes \sigma^3)} \frac{\tilde{g} (\hat{Q} \otimes \sigma^3) \tilde{g}^{-1}}{\tilde{I} + \exp(-\beta \hat{E} \otimes \sigma^3)} \right),$$

etc.

Equations (6.26), (6.27) are obtained with the help of (6.24), (6.25), i.e., from the integral representations of the type (6.1). As an additional check of consistency between (6.24), (6.25), on the one hand, and the results given by finite-dimensional determinants deduced in Subsection 6.1, on the other, one can verify that appropriate differentiations of $\det(\widehat{\delta} + \widehat{M}_F(\alpha))$ (6.6) (with $\widehat{M}_F(\alpha)$ (6.7b)) over α also result in (6.26). Similarly, differentiations of $\det^{1/2}(\widehat{I} + \widehat{M}_F(\alpha))$ (6.12), where $\widehat{M}_F(\alpha)$ is given by (6.19c), also lead us to (6.27).

As an other example, let us calculate, in the thermodynamic limit, the derivatives $(G_F^\pm)'_\alpha$ and $(G_F^\pm)''_\alpha$ at $\alpha = 0$ using, for a comparison, (6.12) and (6.17). To proceed, we adopt the following definitions:

$$C_q \equiv 1 - \cos \theta_q \operatorname{th} \frac{\beta E_q}{2}, \quad S_q \equiv \sin \theta_q \operatorname{th} \frac{\beta E_q}{2}. \quad (6.28)$$

It is straightforward to establish the following relation:

$$\begin{aligned} \left. \frac{d}{d\alpha} G_F^\pm \right|_{\alpha=0} &= \operatorname{tr} \left(\widehat{K}'_F(0) \right) \\ &= \frac{1}{2} \left[m + \operatorname{tr} \left(\widetilde{M}'_F(0) \right) \right] = \frac{m}{2} \int_{-\pi}^{\pi} C_q \frac{dq}{2\pi}, \end{aligned} \quad (6.29)$$

where C_q is given by (6.28). Further,

$$\left. \frac{d^2}{d\alpha^2} G_F^\pm \right|_{\alpha=0} = \operatorname{tr}^2 \left(\widehat{K}'_F(0) \right) + \operatorname{tr} \left(\widehat{K}''_F(0) \right) - \operatorname{tr} \left(\widehat{K}'_F(0) \widehat{K}'_F(0) \right) \quad (6.30a)$$

$$= \frac{1}{4} \left[m + \operatorname{tr} \left(\widetilde{M}'_F(0) \right) \right]^2 + \frac{1}{2} \operatorname{tr} \left(\widetilde{M}''_F(0) \right) - \frac{1}{2} \operatorname{tr} \left(\widetilde{M}'_F(0) \widetilde{M}'_F(0) \right). \quad (6.30b)$$

We take into account that $\operatorname{tr} \left(\widetilde{M}''_F(0) \right) = m$, $\operatorname{tr} \left(\widehat{K}''_F(0) \right) = \operatorname{tr} \left(\widehat{K}'_F(0) \right)$, and

$$\begin{aligned} -\frac{1}{2} \operatorname{tr} \left(\widetilde{M}'_F(0) \widetilde{M}'_F(0) \right) &= -\frac{m}{2} \int_{-\pi}^{\pi} \cos \theta_q \operatorname{th} \frac{\beta E_q}{2} \frac{dq}{2\pi} \\ &+ \frac{1}{4} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} Q_{pq} Q_{qp} (S_p S_q - C_p C_q) dp dq, \end{aligned}$$

where C_q and S_q are given by (6.28). Then, direct use of explicit form of $\widehat{K}'_F(0)$ to express $\operatorname{tr} \left(\widehat{K}'_F(0) \widehat{K}'_F(0) \right)$ in (6.30a) demonstrates us that (6.30a) and (6.30b) coincide.

To conclude the section, let us use the obtained formulas (6.29), (6.30) to calculate the correlators $\langle \sigma_m^z \rangle$ and $\langle \sigma_{m+1}^z \sigma_1^z \rangle$ in the thermodynamic limit. In this case, the contributions $G_B^+ Z_B^+$ and $G_B^- Z_B^-$ in (2.9) cancel and only derivatives of G_F^\pm are important. We obtain for $\langle Q^n(m) \rangle$:

$$\langle Q(m) \rangle = \frac{m}{4\pi} \int_{-\pi}^{\pi} C_q dq, \quad \langle Q^2(m) \rangle = \frac{m}{4\pi} \int_{-\pi}^{\pi} C_q dq + \left(\frac{m}{4\pi} \int_{-\pi}^{\pi} C_q dq \right)^2$$

$$+\frac{1}{4}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}Q_{pq}Q_{qp}(S_pS_q-C_pC_q)dpdq, \quad (6.31)$$

where C_q, S_q are given by (6.28). The usage of (6.20) instead of (6.12) also leads to (6.31). The relations obtained lead to the correct answers for the correlation functions [4], [10], [11]:

$$\langle\sigma_m^z\rangle=(1/2\pi)\int_{-\pi}^{\pi}\cos\theta_q\operatorname{th}\frac{\beta E_q}{2}dq, \quad (6.32)$$

where the definitions

$$\langle\sigma_m^z\rangle=1-2\mathcal{D}_1\langle Q(m)\rangle$$

and $\mathcal{D}_1f(m)=f(m)-f(m-1)$ are used. We obtain further:

$$\langle\sigma_{m+1}^z\sigma_1^z\rangle-\langle\sigma_m^z\rangle^2=(1/4\pi^2)\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos m(p-q)(S_pS_q-C_pC_q)dpdq, \quad (6.33)$$

where the definitions

$$\langle\sigma_{m+1}^z\sigma_1^z\rangle=2\mathcal{D}_2\langle Q^2(m)\rangle+2\sigma_z-1$$

and $\mathcal{D}_2f(m)=f(m+1)-2f(m)+f(m-1)$ are used.

In the XX -case we obtain, say, from (6.26):

$$\langle Q(m)\rangle=\frac{m}{2\pi}\int_{-\pi}^{\pi}(1+e^{\beta\varepsilon_q})^{-1}dq, \quad (6.34)$$

$$\begin{aligned} \langle Q^2(m)\rangle &= \frac{m}{2\pi}\int_{-\pi}^{\pi}(1+e^{\beta\varepsilon_q})^{-1}dq + \left(\frac{m}{2\pi}\int_{-\pi}^{\pi}(1+e^{\beta\varepsilon_q})^{-1}dq\right)^2 - \\ &\quad - \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}Q_{pq}^2(1+e^{\beta\varepsilon_p})^{-1}(1+e^{\beta\varepsilon_q})^{-1}dpdq. \end{aligned} \quad (6.35)$$

One obtains from (6.34) in the thermodynamic limit:

$$\sigma^z \equiv \langle\sigma_m^z\rangle = 1 - \frac{1}{\pi}\int_{-\pi}^{\pi}\frac{dq}{1+e^{\beta\varepsilon_q}}, \quad (6.36)$$

The result (6.36) agrees with the magnetization $M_z = -\partial F/\partial h$, which is calculated by means of F (5.12). We obtain from (6.35) ($m > 0$):

$$\langle\sigma_{m+1}^z\sigma_1^z\rangle = (\sigma^z)^2 - \frac{1}{\pi^2}\left|\int_{-\pi}^{\pi}\frac{e^{imq}}{1+e^{\beta\varepsilon_q}}dq\right|^2. \quad (6.37)$$

Equations (6.32), (6.33) reproduce (6.36), (6.37) in the limit $\gamma \rightarrow 0$, i.e., at $\theta_q \rightarrow 0$ in C_q, S_q . The answers obtained (6.32), (6.33) agree with the results of [4], [10], [11], [15]. Therefore they witness in favour of self-consistency of the functional-integral representations, given by (3.12) (to be used in (2.9)) with the corresponding boundary conditions, which appear when calculating, in the way inspired by [24], the generating

functional $G(\alpha, m)$ (2.1) for the XY and XX Heisenberg cyclic chains. The boundary conditions in the imaginary time which follow (3.12) are given by (3.8) (for $G_F^\pm Z_F^\pm$) and by (3.13) (for $G_B^\pm Z_B^\pm$). Besides, our regularizations resulting in the general expressions (6.6), (6.7), (6.12), (6.19) look satisfactory since final results agree with the results obtained by other methods.

7 Discussion

The generating functionals of static correlators of third components of local spins for the XY and XX Heisenberg spin $1/2$ chains are calculated in the present paper. The calculation is carried out by means of the functional integration over trajectories with “automorphic” dependence on the imaginary time. The results are obtained in the form of determinants of the matrix operators which are regularized by means of zeta-regularization. It is demonstrated that, from a practical standpoint (i.e., if only differentiations over the parameter α are needed), the formula for the first derivative over α of the generating functional can be obtained without regularization of the Mellin integral at the lower bound. Various special limits are considered for the formulas obtained which demonstrate reductions of the XY -case to the known relations of the XX -case.

The given paper continues [23] where a method has been proposed which allows to calculate vacuum average of an exponential of quadratic operator as a functional integral over “automorphic” trajectories. The present paper is close to [24] where the functional integration with “automorphic” boundary conditions is used for a calculation of certain differential geometric indices. The present paper is also close to [27], where the partition functions of spin $1/2$ and spin 1 chain models have been also obtained in the form of path integrals over variables subjected to “automorphic” boundary conditions. The distinction of the present paper from [24], [27] consists in the fact the “automorphic” boundary condition in the imaginary time appears only for a part of sites. The method proposed in [23] is considered above for the system which is equivalent to quasi-free fermions (i.e., the corresponding Hamiltonian is diagonalized by the Bogoliubov transformation). Approach presented provides further development of the technical finds discussed in [24], [27], [28], and it seemingly merits attention since can be used further, for instance, for the XX Heisenberg model with translationally inhomogeneous boundary conditions. In general, the functional integral considered merits attention since it can be useful, as a technical method, for other models where it is also necessary to calculate vacuum averages of exponentials of quadratic operators of the type of $\exp(\alpha Q(m))$.

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NOTE ADDED IN PROOF:

Equation (6.18) demonstrates, in fact, that the square root in G_F^\pm (6.12) can be calculated at $\gamma = 0$ thus leading to an expression in the form of the determinant of the matrix of the size $M \times M$. The same is true for $\gamma \neq 0$ also: calculation of the square root in (6.12) at $\gamma \neq 0$ leads to G_F^\pm just in the form (6.17). The corresponding details should be presented elsewhere.